

Geometric magnetism in open quantum systems

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An isolated classical chaotic system, when driven by the slow change of several parameters, responds with two reaction forces: geometric friction and geometric magnetism. By using the theory of quantum fluctuation relations we show that this holds true also for open quantum systems, and provide explicit expressions for those forces in this case. This extends the concept of Berry curvature to the realm of open quantum systems. We illustrate our findings by calculating the geometric magnetism of a damped charged quantum harmonic oscillator transported along a path in physical space in presence of a magnetic field and a thermal environment. We find that in this case the geometric magnetism is unaffected by the presence of the heat bath.

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I. INTRODUCTION

According to the adiabatic theorem, when a thermally isolated quantum system is subjected to an adiabatic cyclical driving it returns to the same state where it started from [1]. The only effect of the excursion is that the state acquires a phase. In 1984, Berry clarified that such a phase consists of a gauge-dependent (hence non-physical) part and a gauge-independent (hence physical and measurable) part, which is determined only by the geometry of the path described by the driving parameters [2]. This is by now customarily called Berry's phase. Soon later Hannay [3] and Berry [4] found the analogous classical phenomenon: when a classical integrable system undergoes an adiabatic cyclic evolution, the action variable remains constant, but the angle variable experiences an anholonomy effect, that is, it does not return to its original value but accumulates a shift, known as Hannay angle. More recently, Robbins and Berry [5] addressed the question of whether there exists a geometric phase also in the case of classical chaotic systems. Their approach was based on the observation that the Berry phase is given by the flux of a two-form (Berry's curvature) through a surface bounded by the cyclic path in the parameter space. Therefore, they investigated the classical limit of the quantum two-form and found the expression [5]:

$$\mathcal{B}^c = \frac{1}{2\omega(E)} \frac{\partial}{\partial E} \left[\omega(E) \int_0^\infty dt \langle \nabla H_{t=0} \times \nabla H_t \rangle_E \right], \quad (1)$$

where ∇H_t is the gradient in parameter space of the Hamiltonian evaluated at time t (i.e., the instantaneous negative force exerted by the external driving), \times denotes cross product, $\langle \dots \rangle_E$ denotes microcanonical average at energy E and $\omega(E)$ is the corresponding density of states. Later Jarzynski [6] showed that the surface integral of the classical chaotic two-form (1) measures a shift accumulated along the chaotic trajectory on the constant energy hyper-surface, which generalizes the concept of Hannay's angle. In a subsequent paper Berry and Robbins [7] re-derive Eq. (1) adopting a statistical mechanical approach. They considered an initially microcanon-

ically distributed ensemble and focused on the average force with which the system reacts to the external driving, $\mathbf{F} = -\langle \nabla H \rangle_E$, up to first order in the driving speed. They showed that the reaction force contains two terms: a friction-like force and a Lorentz-like force. The latter stems from a magnetic-like field, the so called geometric magnetism, which is nothing but the classical chaotic two-form detailed in Eq. (1). The approach developed in [7] is similar to Kubo's Linear Response Theory [8]. The main differences are: (i) in Kubo's theory the initial state is canonical whereas in Berry and Robbins theory it is microcanonical; (ii) Kubo's theory gives the response of a driven system to a *weak* perturbation, and gives, accordingly, a linear relationship between the response and the strength of the driving. The theory of Berry and Robbins instead yields the response of a driven system to a *slow* perturbation, and gives, accordingly, a linear relationship between the response and the *speed* of the driving. We might label Berry and Robbins theory [7] a *Microcanonical Adiabatic Linear Response Theory*.

In the recent years yet further attempts have been devoted to investigate possible generalizations of Berry's phase. It has been realized that geometric phases can be used as effective and reliable tools for quantum computation [9, 10]. Thus, the study of geometric phases in realistic open quantum systems has become of paramount importance. This problem has been typically addressed from a *dynamics* point of view, that is, one researches proper definitions of phases with respect to non-unitary dynamics [11–21] (which are the relevant ones for open systems), instead of the unitary dynamics originally considered by Berry.

To the best of our knowledge, however, the problem of finding the geometric phase of an open quantum systems was not previously addressed adopting a statistical mechanical method akin to the one employed by Berry and Robbins [7]. Here we pursue this task. Below we develop a *Canonical Adiabatic Linear Response Theory* for open quantum systems. As a main result we obtain the general expression of the field of geometric magnetism of open quantum systems, see Eq. (21) below. The geometric phase is given by its surface integral in analogy

with the standard case. In developing the theory we take full advantage from the theory of quantum work fluctuation relations [22, 23], which can be formulated within two complementary viewpoints: exclusive and inclusive [24, 25]. While the former is best suited to derive Kubo's Linear Response Theory [26, 27], the latter, as we will see below, is best suited to derive the searched Canonical Adiabatic Linear Response Theory.

II. ADIABATIC LINEAR RESPONSE OF OPEN QUANTUM SYSTEMS

We consider a driven open quantum system in contact with a thermal bath at fixed temperature $T = 1/(k_B\beta)$. Following the established procedure [28, 29] we hence close the system by coupling it to a thermal bath. The total (system+bath) Hamiltonian reads

$$\mathcal{H}(\mathbf{R}_t) = H_B + H_{SB} + H(\mathbf{R}_t), \quad (2)$$

where H_B is the bath Hamiltonian, H_{SB} is the (possibly strong) system/bath coupling, and $H(\mathbf{R}_t)$ is the system Hamiltonian:

$$H(\mathbf{R}_t) = H_0 - \mathbf{R}_t \cdot \mathbf{Q}. \quad (3)$$

Here t is time, $\mathbf{R}_t = (R_t^1, \dots, R_t^N)$ denotes a set of time dependent external parameters, (the generalized “displacements”) $\mathbf{Q} = (Q^1, \dots, Q^N)$ is the set of conjugated system observables (the generalized “forces”), and “ \cdot ” denotes the scalar product. We assume that the bath is *ideal*, meaning that it has infinite heat capacity C and, accordingly, cannot change its temperature T upon injection of finite amounts of energy. For convenience we introduce the notations

$$\varrho_{\mathbf{R}}^{\text{eq}} = e^{-\beta\mathcal{H}(\mathbf{R})}/\mathcal{Z}_{\mathbf{R}}, \quad \mathcal{Z}_{\mathbf{R}} = \text{Tr} e^{-\beta\mathcal{H}(\mathbf{R})}, \quad (4)$$

to denote the Gibbs equilibrium of the total system at fixed parameters \mathbf{R} , and the corresponding partition function (Tr is the trace over the total system). We assume that at $t = 0$ the total system is in the equilibrium $\varrho_{\mathbf{R}_0}^{\text{eq}}$. We next consider some system observable O , and ask how its expectation value at time $t = \tau$,

$$\langle O_\tau \rangle \doteq \text{Tr} \varrho_{\mathbf{R}_0}^{\text{eq}} O_\tau = \text{Tr} \varrho_\tau O, \quad (5)$$

deviates from its equilibrium expectation value

$$\langle O \rangle_{\mathbf{R}_\tau}^{\text{eq}} \doteq \text{Tr} \varrho_{\mathbf{R}_\tau}^{\text{eq}} O. \quad (6)$$

Here, O_τ denotes the Heisenberg picture $O_t = U_{t0}^\dagger O U_{t0}$, ϱ_t is the total system density matrix at time t : $\varrho_t = U_{t0} \varrho_{\mathbf{R}_0}^{\text{eq}} U_{t0}^\dagger$, and $U_{\tau t}$ denotes the quantum time evolution operator from time t to time τ , generated by the total Hamiltonian $\mathcal{H}(\mathbf{R}_t)$.

Using the cyclic property of the trace operator, and the property $U_{\tau t}^\dagger U_{\tau t} = \mathbb{1}$, one can prove the following nonequilibrium identity

$$\langle O_\tau e^{-\beta\mathcal{H}_\tau(\mathbf{R}_\tau)} e^{\beta\mathcal{H}_0(\mathbf{R}_0)} \rangle_{\mathbf{R}_0}^{\text{eq}} = e^{-\beta\Delta F} \langle O \rangle_{\mathbf{R}_\tau}^{\text{eq}}, \quad (7)$$

where $\Delta F = -\beta^{-1} \ln(\mathcal{Z}_{\mathbf{R}_\tau}/\mathcal{Z}_{\mathbf{R}_0})$ is the difference of free energy of the total system states $\varrho_{\mathbf{R}_\tau}^{\text{eq}}$ and $\varrho_{\mathbf{R}_0}^{\text{eq}}$. For $O = \mathbb{1}$ Eq. (7) reproduces the quantum Jarzynski Equality [22, 30]. Eq. (7) may be obtained from the nonequilibrium generating functional of Andrieux and Gaspard [27] by means of functional differentiation. Note that the free energy difference can be written in the following form [31]: $\Delta F = -\int_{\mathbf{R}_0}^{\mathbf{R}_\tau} d\mathbf{R} \cdot \langle \mathbf{Q} \rangle_{\mathbf{R}}^{\text{eq}} = -\int_0^\tau dt \dot{\mathbf{R}}_t \cdot \langle \mathbf{Q} \rangle_{\mathbf{R}_t}^{\text{eq}}$. Using the notations

$$W = \mathcal{H}_\tau(\mathbf{R}_\tau) - \mathcal{H}(\mathbf{R}_0) = -\int_0^\tau dt \dot{\mathbf{R}}_t \cdot \mathbf{Q}_t, \quad (8)$$

$$W_{\text{dis}} = W - \Delta F = -\int_0^\tau dt \dot{\mathbf{R}}_t \cdot [\mathbf{Q}_t - \langle \mathbf{Q} \rangle_{\mathbf{R}_t}^{\text{eq}}], \quad (9)$$

Eq. (7) reads:

$$\langle O_\tau e^{-\beta\mathcal{H}_\tau(\mathbf{R}_\tau)} e^{\beta[\mathcal{H}_\tau(\mathbf{R}_\tau) - W_{\text{dis}}]} \rangle_{\mathbf{R}_0}^{\text{eq}} = \langle O \rangle_{\mathbf{R}_\tau}^{\text{eq}}. \quad (10)$$

The operators W and W_{dis} do not correspond to any quantum-mechanical observable [22, 30], but approach, – in the classical limit –, the exclusive work, w , and dissipated work, $w - \Delta F$, respectively [25]. Under our assumptions that the bath has infinite heat capacity, the nonequilibrium expectation (5) of W_{dis} vanishes in the adiabatic limit (for a discussion of the scaling of W_{dis} with the bath size in a classical set-up, see [32]). Since the expectation of W_{dis} is given by the Kullback-Leibler relative entropy between ϱ_τ and $\varrho_{\mathbf{R}_\tau}^{\text{eq}}$ [33–36], this also means that in the adiabatic limit $\varrho_\tau \rightarrow \varrho_{\mathbf{R}_\tau}^{\text{eq}}$. As the driving speed increases, the actual state ϱ_τ lags more and more behind the “reference” equilibrium state $\varrho_{\mathbf{R}_\tau}^{\text{eq}}$ [32].

In the following we consider slow (quasi-adiabatic) driving, and accordingly expand Eq. (10) to first order in W_{dis} (here slow means that the characteristic time of variation of the driving is small compared to the characteristic time of relaxation to the Gibbs equilibrium). Following the method outlined in Ref. [27], we use the operator expansion:

$$e^{\beta A} e^{-\beta(A-\epsilon)} = 1 + \int_0^\beta du e^{uA} \epsilon e^{-uA} + O(\epsilon^2). \quad (11)$$

Setting $A = -\mathcal{H}_\tau(\mathbf{R}_\tau)$ and $\epsilon = -W_{\text{dis}}$, we arrive, to first order in W_{dis} , at the result

$$\begin{aligned} \langle \Delta O_\tau \rangle &\doteq \langle O_\tau \rangle - \langle O \rangle_{\mathbf{R}_\tau}^{\text{eq}} \\ &= -\int_0^\tau dt \int_0^\beta du \langle O_\tau e^{-u\mathcal{H}_\tau(\mathbf{R}_\tau)} \Delta \mathbf{Q}_t e^{u\mathcal{H}_\tau(\mathbf{R}_\tau)} \cdot \dot{\mathbf{R}}_t \rangle_{\mathbf{R}_0}^{\text{eq}}. \end{aligned} \quad (12)$$

Using the cyclic property of the trace operator and unitarity $U_{\tau t}^\dagger U_{\tau t} = \mathbb{1}$, we rewrite the integrand in Eq. (12) as:

$$\text{Tr} \varrho_\tau O U_{\tau 0} e^{-u\mathcal{H}(\mathbf{R}_\tau)} U_{\tau t} \Delta \mathbf{Q} U_{\tau t}^\dagger e^{u\mathcal{H}(\mathbf{R}_\tau)} U_{\tau 0}^\dagger \cdot \dot{\mathbf{R}}_t. \quad (13)$$

Since this expression is already of first order in W_{dis} we can replace the exact density matrix ϱ_τ with the approximate equilibrium density matrix $\varrho_{\mathbf{R}_\tau}^{\text{eq}}$. The next, crucial

assumption is that the correlation function in Eq. (12) decays quickly compared to the time scale of variation of \mathbf{R}_t , which, in fact was assumed to be very large. Under this assumption, one can approximate the exact time evolution operator $U_{\tau t}$ with the time evolution at frozen $\mathbf{R} = \mathbf{R}_\tau$: $U_{\tau t} \simeq e^{-i\mathcal{H}(\mathbf{R}_\tau)(t-\tau)/\hbar}$, replace \mathbf{R}_t by \mathbf{R}_τ , to arrive at:

$$\langle \Delta O_\tau \rangle = - \sum_i \int_0^\tau dt \Phi_{i,O}^{\mathbf{R}_\tau}(t-\tau) \dot{R}_\tau^i \quad (14)$$

$$\Phi_{i,O}^{\mathbf{R}_\tau}(t) \doteq \int_0^\beta du \langle \Delta O_{-i\hbar u} \Delta Q_t^i \rangle_{\mathbf{R}_\tau}^{\text{eq}}. \quad (15)$$

Note that $\Phi_{i,O}^{\mathbf{R}_\tau}(t)$ is the quantum equilibrium correlation function between O and ΔQ^i (i.e., the relaxation function [8]) calculated with respect to the equilibrium state and propagator at fixed $\mathbf{R} = \mathbf{R}_\tau$.

III. GEOMETRIC FRICTION AND GEOMETRIC MAGNETISM

The theory applies regardless of the number N of driving parameters. Geometric magnetism only appears in the case where there are at least $N \geq 2$ driving parameters.

Choosing O as the i -th component of the force, Q^i , Eq. (12) becomes, using vector notation:

$$\langle \Delta \mathbf{Q}_\tau \rangle = -\mathbf{K}(\mathbf{R}_\tau) \dot{\mathbf{R}}_\tau, \quad (16)$$

where $\mathbf{K}(\mathbf{R}_\tau)$ is the $N \times N$ conductance matrix whose elements are the integrated force-force equilibrium correlation functions:

$$\begin{aligned} K^{jk}(\mathbf{R}_\tau) &= \int_0^\tau dt \int_0^\beta du \langle \Delta Q_{-i\hbar u}^j \Delta Q_{t-\tau}^k \rangle_{\mathbf{R}_\tau}^{\text{eq}} \\ &= \int_0^\tau dt \left(\int_0^\beta du \langle Q_{-i\hbar u}^j Q_{t-\tau}^k \rangle_{\mathbf{R}_\tau}^{\text{eq}} - \langle Q^j \rangle_{\mathbf{R}_\tau}^{\text{eq}} \langle Q^k \rangle_{\mathbf{R}_\tau}^{\text{eq}} \right). \end{aligned} \quad (17)$$

$$(18)$$

Note that the r.h.s of Eqs. (14, 16) are geometric, i.e., they depend on time only through the time dependent parameters \mathbf{R}_τ . Following Berry and Robbins [7] we assume for simplicity a parameter space of dimension $N = 3$ and rewrite Eq. (16) in vector notation as:

$$\langle \Delta \mathbf{Q}_\tau \rangle = -\mathbf{K}^S(\mathbf{R}_\tau) \dot{\mathbf{R}}_\tau - \mathbf{B}(\mathbf{R}_\tau) \times \dot{\mathbf{R}}_\tau. \quad (19)$$

The first term, stemming from the symmetric part \mathbf{K}^S of the conductance matrix \mathbf{K} , is *geometric friction*, and the second term, stemming from the antisymmetric part \mathbf{K}^A of the conductance matrix is *geometric magnetism*. The field of geometric magnetism, \mathbf{B} , has components $B_i = -1/2 \sum_{jk} \varepsilon_{ijk} K^{jk}$ [ε_{ijk} is the Levi-Civita tensor], and reads, in vector notation:

$$\mathbf{B}(\mathbf{R}_\tau) = -1/2 \int_0^\tau dt \int_0^\beta du \langle \mathbf{Q}_{-i\hbar u} \times \mathbf{Q}_{t-\tau} \rangle_{\mathbf{R}_\tau}^{\text{eq}}. \quad (20)$$

The theory may be generalized to account for general *nonlinear* driving, i.e., to system Hamiltonians $H(\mathbf{R}_t)$ not necessarily of the form in Eq. (3). In the general case the operator W reads [24]: $W = \int_0^\tau dt \dot{\mathbf{R}}_t \cdot \nabla H_t(\mathbf{R}_t)$. Accordingly, the general theory is obtained by replacing everywhere \mathbf{Q} with ∇H . A main result, therefore, is that the field of geometric magnetism emerges as:

$$\mathbf{B}(\mathbf{R}) = 1/2 \int_0^\infty dt \int_0^\beta du \langle \nabla H_{-i\hbar u} \times \nabla H_t \rangle_{\mathbf{R}}^{\text{eq}}. \quad (21)$$

where for simplicity we have changed the integration domain from $[0, \tau]$ to $(-\infty, 0]$, we have used the fact that the antisymmetric part of the relaxation function is odd under $t \rightarrow -t$ [8] to express the result as an integral from 0 to ∞ , and we have dropped the time label $\tau = 0$ in \mathbf{R} . Eq. (21) is the *open quantum system* version of Berry and Robbins expression (1) for the geometric magnetism of an isolated classical chaotic system.

It is worthwhile to re-express Eq. (21) in terms of the symmetrized force autocorrelation function

$$\Psi_{jk}^{\mathbf{R}}(t) = 1/2 \langle \{ \partial_k H, \partial_j H_t \} \rangle_{\mathbf{R}}^{\text{eq}}, \quad (22)$$

where $\{\cdot, \cdot\}$ denotes quantum anti-commutator and $\partial_j = \partial/\partial R_j$. To this end we rewrite it in tensor notation as

$$\mathcal{B}_i(\mathbf{R}) = (-1/2) \sum_{jk} \varepsilon_{ijk} \int_0^\infty dt \Phi_{jk}^{\mathbf{R}}(t), \quad (23)$$

where $\Phi_{jk}^{\mathbf{R}}(t)$ is the relaxation function between $\partial_j H$ and $\partial_k H$, see Eq. (15). According to the fluctuation-dissipation theorem [8]

$$\Phi_{jk}^{\mathbf{R}}(t) = \int_{-\infty}^\infty dt' \Gamma(t-t') \Psi_{jk}^{\mathbf{R}}(t') \quad (24)$$

$$\Gamma(t) = \frac{2}{\hbar\pi} \ln \left[\coth \left(\frac{\pi|t|}{2\beta\hbar} \right) \right], \quad (25)$$

hence

$$\mathcal{B}_i(\mathbf{R}) = -1/2 \sum_{jk} \varepsilon_{ijk} \int_0^\infty dt \int_{-\infty}^{+\infty} dt' \Gamma(t-t') \Psi_{jk}^{\mathbf{R}}(t'), \quad (26)$$

or, in vector notation:

$$\begin{aligned} \mathbf{B}(\mathbf{R}) &= 1/4 \int_0^\infty dt \int_{-\infty}^{+\infty} dt' \Gamma(t-t') \\ &\quad \langle \nabla H \times \nabla H_{t'} - \nabla H_{t'} \times \nabla H \rangle_{\mathbf{R}}^{\text{eq}}. \end{aligned} \quad (27)$$

Eq. (23) can be re-written in a remarkably simple form:

$$\mathcal{B}_i(\mathbf{R}) = (-1/2) \sum_{jk} \varepsilon_{ijk} \tilde{\Phi}_{jk}^{\mathbf{R}}(0), \quad (28)$$

where the symbol $\tilde{\Phi}_{jk}^{\mathbf{R}}(s) = \int_0^\infty dt e^{-st} \Phi_{jk}^{\mathbf{R}}(t)$ denotes the Laplace transform of $\Phi_{jk}^{\mathbf{R}}(t)$.

Classical limit

Eq. (16) holds true also classically. The derivation can be repeated following the quantum derivation given above, allowing observables to commute. As a result, the quantum thermal correlation functions have to be replaced by the classical expressions [8], so that the classical geometric magnetism reads:

$$\mathcal{B}^{\text{cl}}(\mathbf{R}) = \beta/2 \int_0^\infty dt \langle \nabla H \times \nabla H_t \rangle_{\mathbf{R}}^{\text{eq}}. \quad (29)$$

This result may also be obtained by taking the limit $\hbar \rightarrow 0$ of Eq. (21). Alternatively one can take the limit $\hbar \rightarrow 0$ of Eq. (27). In this limit $\Gamma(t) \rightarrow \beta\delta(t)$ [8], where δ denotes Dirac's delta function, and observables commute $\nabla H_{t'} \times \nabla H \rightarrow -\nabla H \times \nabla H_{t'}$.

IV. OPEN SYSTEM DYNAMICS

The geometric magnetism (and the geometric friction too) may be recast in the more familiar language of *dissipative open system dynamics* [37, 38], in terms of the system reduced density matrix

$$\rho_\tau^S = \text{Tr}_B \rho_\tau, \quad (30)$$

where Tr_B denotes the trace over the bath Hilbert space. The linear response of the force, which defines the conductance matrix \mathbf{K} (hence the geometric friction and the geometric magnetism), may be written as:

$$\begin{aligned} \langle \Delta Q_\tau \rangle &= \text{Tr} \rho_\tau Q - \text{Tr} \rho_{\mathbf{R}_\tau}^{\text{eq}} Q \\ &= \text{Tr}_S \rho_\tau^S Q - \langle Q \rangle_{\mathbf{R}_\tau}^{\text{eq}, S}, \end{aligned} \quad (31)$$

where Tr_S denotes the trace over the system- S Hilbert space and $\langle \cdot \rangle_{\mathbf{R}_\tau}^{\text{eq}, S}$ denotes expectation over the equilibrium reduced density matrix [39]

$$\rho_{\mathbf{R}}^{\text{eq}, S} = \text{Tr}_B e^{-\beta \mathcal{H}(\mathbf{R})} / Z_{\mathbf{R}} = e^{-\beta H^*(\mathbf{R})} / Z_{\mathbf{R}}, \quad (32)$$

where $H^*(\mathbf{R})$ is the Hamiltonian of mean force and $Z_{\mathbf{R}} = \text{Tr}_S e^{-\beta H^*(\mathbf{R})}$ is the partition function of an open quantum system [29, 37–39]. In the case of weak coupling the Hamiltonian of mean force reduces to the system Hamiltonian H_S .

The element K^{jk} of the conductance matrix may be experimentally/numerically obtained by driving the system with a small constant velocity in the \hat{j} direction, $V_j \hat{j}$ and measuring/computing the reaction force in the k direction:

$$K^{jk}(\mathbf{R}_\tau) = - \left[\text{Tr}_S \rho_\tau^{S,j} Q_k - \langle Q_k \rangle_{\mathbf{R}_\tau}^{\text{eq}, S} \right] / V_j, \quad (33)$$

where we have introduced the notation $\rho_\tau^{S,j}$ to denote the reduced density matrix resulting from the perturbation $V_j \hat{j}$. Accordingly, the geometric magnetism may be

expressed in terms of the reduced density matrix

$$\mathcal{B}_i(\mathbf{R}_\tau) = 1/2 \sum_{jk} \varepsilon_{ijk} \left[\text{Tr}_S \rho_\tau^{S,j} Q_k - \langle Q_k \rangle_{\mathbf{R}_\tau}^{\text{eq}, S} \right] / V_j. \quad (34)$$

As illustrated above the geometric magnetism may be accessed also by calculating the equilibrium force autocorrelation function. Although quantum correlation functions can not in general be expressed as expectations over the reduced density matrix, they are “open quantum systems” objects that depend explicitly on bath properties, notably the bath spectral density, see Eq. (39) below. In particular, it should be noted that exact open quantum system dynamics generally is (i) neither linear [40] (ii) nor can it be described by trace preserving completely positive maps [41, 42]. Attempts to resort to approximations (e.g. Markov, and rotating wave) to express the correlation functions in terms of Markovian dynamics for the system observables, may lead to results which contradict basic principles such as the fluctuation dissipation theorem [43], and therefore to non-negligible errors in the evaluation of geometric friction and magnetism. See Ref. [44] for a recent example of the drastic effects that even good approximations may have on the calculation of geometric phases. Therefore a very special care must be paid when employing such approximations in this context.

V. ILLUSTRATION: THE DAMPED CHARGED HARMONIC OSCILLATOR IN A MAGNETIC FIELD

As an illustration of the theory we consider a quantum damped charged harmonic oscillator of mass m and charge q transported along a path \mathbf{R}_t in presence of a constant magnetic field \mathbf{B} . Adopting the Caldeira-Leggett model of quantum Brownian motion [45], the system, bath and coupling Hamiltonian read:

$$\begin{aligned} H(\mathbf{R}_t) &= (\mathbf{p} - q\mathbf{A})^2 / (2m) + m\omega^2 \mathbf{x}^2 / 2 - m\omega^2 \mathbf{x} \cdot \mathbf{R}_t \\ H_B &= \sum_{n=1}^N [\mathbf{P}_n^2 / m_n + m_n \omega_n^2 \boldsymbol{\xi}_n^2] / 2 \\ H_{SB} &= -\mathbf{x} \cdot \sum_{n=1}^N c_n \boldsymbol{\xi}_n + \mathbf{x}^2 \sum_{n=1}^N c_n / (2m_n \omega_n^2). \end{aligned} \quad (35)$$

Here $\mathbf{x}, \mathbf{p}, \omega$ denote the harmonic oscillator position, momentum and frequency, respectively. $\boldsymbol{\xi}_n, \mathbf{P}_n, m_n, \omega_n$ denote the n th bath's oscillator position, momentum, mass and frequency, respectively. The symbol c_n denotes the linear coupling constant between the harmonic oscillator and the n th bath's oscillator. The symbol \mathbf{A} denotes the vector potential. Note that according to Eq. (3) $\mathbf{Q} = m\omega^2 \mathbf{x}$. Assuming an initial global Gibbs distribution and adopting the Feynmann-Vernon path integral approach [37] one arrives, after integrating out the bath's degrees of freedom, at the following generalized quantum

Langevin equation for the charged oscillator's position [46]

$$m\ddot{\mathbf{x}}_t + \int_{-\infty}^t dt' \eta(t-t') \dot{\mathbf{x}}_{t'} - q\dot{\mathbf{x}}_t \times \mathbf{B} + m\omega^2 \mathbf{x}_t = \mathbf{F}_t + \mathbf{f}_t, \quad (36)$$

where $\eta(t)$ is the friction kernel, $\mathbf{f}_t = m\omega^2 \mathbf{R}_t$ is the externally applied force, and \mathbf{F}_t is the stochastic force. Without loss of generality we shall assume that \mathbf{B} points in the z direction, $\mathbf{B} = B\hat{\mathbf{z}}$. Since the motion in the z direction is decoupled from the motion in the x and y directions, the xz and yz relaxation functions vanish, implying that the geometric magnetism is also directed in the $\hat{\mathbf{z}}$ direction. Further, due to spatial homogeneity, geometric magnetism does not depend explicitly on the position \mathbf{R}_t . That is, $\mathbf{B} = B\hat{\mathbf{z}}$. From the compact expression (28) the strength of the geometric magnetism reads

$$\mathcal{B} = -1/2[\tilde{\Phi}_{xy}(0) - \tilde{\Phi}_{xy}^a(0)] = -\tilde{\Phi}_{xy}^a(0) \quad (37)$$

where we have introduced the notation Φ_{xy}^a for the anti-symmetric component of Φ_{xy} and $\tilde{\Phi}_{xy}^a(s)$ for its Laplace transform. Following [46] the Laplace transform of the anti-symmetric part of the response function reads

$$\tilde{\alpha}_{xy}^a(s) = \frac{(m\omega^2)^2 qBs}{[m\omega^2 + ms^2 + s\tilde{\eta}(s)]^2 + q^2 B^2 s^2}, \quad (38)$$

where $[\cdot, \cdot]$ denotes quantum commutator, and $\tilde{\eta}(s)$ is the Laplace transform of the bath friction kernel. Its form depends on the bath spectral density. For an ohmic bath $\tilde{\eta}(s)$ is constant. As compared to Eq. (2.15) of Ref. [46], we have in our Eq. (38) an extra factor $(m\omega^2)^2$ stemming from our definition of α_{xy}^a in terms of $Q_x = m\omega^2 x$, $Q_y = m\omega^2 y$, rather than x, y .

Since $\Phi_{xy} = \int_t^\infty dt' \alpha_{xy}(t')$ [8] we have

$$\begin{aligned} \tilde{\Phi}_{xy}^a(s) &= \frac{\tilde{\alpha}_{xy}^a(0)}{s} - \frac{(m\omega^2)^2 qB}{[m\omega^2 + ms^2 + s\tilde{\eta}(s)]^2 + q^2 B^2 s^2} \\ &= -\frac{(m\omega^2)^2 qB}{[m\omega^2 + ms^2 + s\tilde{\eta}(s)]^2 + q^2 B^2 s^2}, \end{aligned} \quad (39)$$

where $\alpha_{xy}^a(0) = 0$ due to the fact that at equal times Q_x and Q_y commute. Regardless of the bath spectral density, the friction kernel $\eta(t)$ vanishes at large times, hence, according to the final value theorem $\lim_{s \rightarrow 0} s\tilde{\eta}(s) = 0$. Using Eq. (37) one finally obtains the result

$$\mathcal{B} = qB, \quad (40)$$

which evidently holds both classically and quantum-mechanically. Apart from the charge q , geometric magnetism is nothing but the physical magnetic field in this case. The factor q stems from the fact that the geometric Lorentz force in Eq. (19) reads $-\mathbf{B} \times \dot{\mathbf{R}}$, whereas the Lorentz force reads $-q\mathbf{B} \times \mathbf{v}$ [where $\mathbf{v} = (\dot{x}, \dot{y}, \dot{z})$]. This

very same result was found also in Refs. [47, 48] for the case of an isolated classical or quantum harmonic oscillator. Our result (40) conveys the non-trivial knowledge that this continues to hold also for an open classical or quantum harmonic oscillator. That is, the presence of a bath does not destroy the geometric magnetism, in fact it does not minimally alter it in this case. Analogous calculations involving the symmetric part of the relaxation function lead to the result that the geometric friction is given by the time integral of the friction kernel $\int_0^\infty dt \eta(t)$.

It is noteworthy that the case of geometric magnetism is distinct from the case of standard equilibrium diamagnetism, which is absent in the classical limit of open systems and reveals itself at the quantum level only, see Bohr-van Leeuwen theorem [49, 50].

VI. CONCLUDING REMARKS

We have derived a general expression for the field of geometric magnetism in open quantum systems, Eq. (21), possibly coupled strongly to the environment. This generalizes the expression (1) of Berry and Robbins [5, 7] which refers to closed chaotic classical systems. It is worth noticing that, contrary to the case studied by Berry and Robbins, here no assumption of chaotic dynamics of the driven system $H(\mathbf{R}_t)$, which may well be integrable, is made. It is the presence of the thermal bath H_B and the coupling to it, H_{BS} , that provide the necessary degree of chaos for the development of a response theory à la Kubo. It is however important to remark the differences between the presently developed theory and that of Kubo. This is best seen by confronting Eq. (14) with Kubo's formula

$$\langle O_\tau \rangle - \langle O \rangle_{\mathbf{R}_0}^{\text{eq}} = \int_0^\tau dt \int_0^{\beta} du \langle \Delta O_{-i\hbar u} \Delta \dot{Q}_{t-\tau} \rangle_{\mathbf{R}_0}^{\text{eq}} \cdot \mathbf{R}_t. \quad (41)$$

Note the prominent difference that Kubo's formula (41) gives an expression (linear in \mathbf{R}) for the difference between the nonequilibrium expectation of O at time τ , and its equilibrium expectation at time 0, whereas the present formula (14) gives an expression (linear in $\dot{\mathbf{R}}$) for the difference between the nonequilibrium expectation of O at time τ , and its equilibrium expectation *at the same time* τ . Thus in Kubo's theory the small parameter is the *strength* of the driving whereas in our theory the small parameter is the *speed*. Both formulae (14, 41) yield the response in terms of equilibrium correlation functions. While Kubo's formula involves the correlation between O and \dot{Q} (the response function), our formula involves the correlation between O and Q (the relaxation function). Note that Kubo's formula (41) follows from an exact fluctuation relation

$$\langle O_\tau e^{-\beta H_{0,\tau}} e^{\beta H_0} \rangle_{\mathbf{R}_0}^{\text{eq}} = \langle O \rangle_{\mathbf{R}_0}^{\text{eq}}, \quad (42)$$

that looks very similar to our starting Eq. (7) [26, 27]. The differences are that (i) the r.h.s. is evaluated at \mathbf{R}_0

in Eq. (42), while it is calculated at \mathbf{R}_τ in Eq. (7), (ii) Eq. (42) does not involve the free energy difference ΔF , which instead appears in Eq. (7), (iii) in Eq. (42) the unperturbed system Hamiltonian H_0 appears instead of the total Hamiltonian $\mathcal{H}(\mathbf{R}_t)$ appearing in Eq. (7). These complementary expressions (7) and (42) are customarily referred to as “inclusive viewpoint” and “exclusive viewpoint” fluctuation relations, respectively. Interested readers can find accounts of the importance of these viewpoints in the theory of nonequilibrium fluctuations in Refs. [22, 24, 25]. Just like Eq. (42) allows one to obtain Kubo’s formula (41) and the whole hierarchy of higher order nonlinear responses, so does Eq. (7) allow to obtain the adiabatic linear response relation (14), as well as the higher order terms in the adiabatic expansion. An interesting open question is whether and under which conditions geometric forces appear in those higher order terms.

Our main result, Eq. (21), provides a straightforward way to define the Berry phase of an open quantum system. Just like the surface integral of the classical two-form (1) provides a generalization of Berry phase for chaotic classical systems [5, 6], so does the surface integral of the geometric magnetism (21) provide an analogue of the Berry phase of open quantum systems, reading

$$\gamma = \int \mathcal{B} \cdot d\mathbf{\Sigma}. \quad (43)$$

This so defined phase γ would in general differ from those, equally sound and useful, expressions of a Berry phase introduced for open systems in the prior literature [11–21]. In full analogy with the original Berry phase, γ is geometric, that is it depends only on the path described by the driving parameters. It vanishes for a path enclosing no area, and it vanishes in the case when the system dynamics are time-reversal invariant, i.e., when for any t , $\Theta \mathcal{H}(\mathbf{R}_t) = \mathcal{H}(\mathbf{R}_t) \Theta$. Here Θ is the anti-unitary time-reversal operator which reverses momenta and keeps the spatial coordinates and all external parameters (possibly

including physical magnetic fields) unaltered [1, 22]. This is so because, due to Onsager-Casimir relations [51], the conductance matrix \mathbf{K} would be symmetric in this case, hence, the geometric magnetism \mathcal{B} would vanish.

Our simple example of a quantum harmonic oscillator transported along a path already shows that the presence of an environment does not destroy geometric magnetism. In fact, in this specific (linear) case the geometric magnetism is given by the actual physical magnetic field, exactly like in the isolated case [47, 48]. For nonlinear systems the difference between the real and geometric magnetic fields could be detected, as well as the difference between quantum and classical regimes. However, the quantum-mechanical treatment of nonlinear open systems constitutes an ambitious challenge because in this case the system evolution cannot be handled analytically in an exact manner. This challenge, in principle, could be approached numerically, for example, (i) by resorting to the Floquet-Markov formalism [52], under the assumption of weak system-bath coupling; or (ii) by following the Feynmann-Vernon path integral formalism [29, 37], to calculate the reduced density matrix numerically, through stochastic unraveling of the corresponding influence functional [53].

Geometric magnetism is at the basis of a currently growing experimental activity aimed at producing *artificial gauge fields* in thermally isolated cold atomic gases [54–58]. The present theory opens the possibility of engineering synthetic gauge fields also in the presence of a thermal environment, via our general expression (21).

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